

## Bayesian Estimation

Thomas Bayes (18th-century mathematician and statistician)

Sir Harold Jeffreys (famous 20th-century mathematician and statistician) wrote:

“Bayes’ theorem is to the theory of probability what Pythagoras’s theorem is to geometry”

### Review: Properties of ML Estimator

Data: i.i.d. sample of size  $N$  drawn from  $P(X|\theta)$

Consistency: As  $N$  increases, the sequence of MLE estimates  $\hat{\theta}(N)$  converges in probability to the true parameter value  $\theta$

Asymptotic Normality: As the sample size increases, the distribution of the MLE tends to the Gaussian distribution with mean  $\theta$  (and covariance matrix equal to the inverse of the Fisher information matrix)

Efficiency: No consistent estimator has lower asymptotic mean squared error than the ML estimator (ML estimator achieves the Cramer-Rao lower bound when the sample size tends to infinity)

### Bayes’ Rule / Theorem

For events  $A$  and  $B$ ,  $P(A|B) = P(B|A)P(A)/P(B)$

Proof follows from our definition of conditional probability, i.e.,  $P(X|Y) := P(X \cap Y)/P(Y)$

### Example (Coin Flip)

Consider that we don’t know if a coin is fair / unfair

We have 2 possibilities in our mind:

(1) Coin fair, i.e.,  $P(\text{head}) = p = 0.5$

(2) Coin biased towards heads with  $P(\text{head}) = q = 0.7$

We have a belief (**prior** to observing data) that  $P(\text{CoinFair}) = 0.8$

Now we experiment with the coin, collect data, and recompute the probability that the coin is fair

$$P(\text{CoinFair}|\text{Data}) = P(\text{Data}|\text{CoinFair})P(\text{CoinFair})/P(\text{Data})$$

Given: We have data =  $n$  observations with  $r$  heads and  $(n - r)$  tails. What does the data do to our belief ?

$$P(\text{Data}|\text{CoinFair}) = C_r^n 0.5^r 0.5^{n-r}$$

$$P(\text{Data}|\text{CoinUnfair}) = C_r^n 0.7^r 0.3^{n-r}$$

$$P(\text{Data}) = P(\text{Data}|\text{CoinFair})P(\text{CoinFair}) + P(\text{Data}|\text{CoinUnfair})P(\text{CoinUnfair})$$

$$P(\text{CoinFair}|\text{Data}) = \frac{0.5^r 0.5^{n-r} \times 0.8}{0.5^r 0.5^{n-r} \times 0.8 + 0.7^r 0.3^{n-r} \times 0.2}$$

Case 1:

If  $n = 20, r = 11$ , then  $P(\text{CoinFair}|\text{Data}) = 0.9074$  which is more than 0.8. So the data has strengthened our belief !  
Why has this happened ? Because 11 heads out of 20 is more like the fair coin.

Case 2:

If  $n = 20, r = 13$ , then  $P(\text{CoinFair}|\text{Data}) = 0.6429$  which is less than 0.8. So the data has weakened our belief !  
Why has this happened ? Because 13 heads out of 20 is more like the unfair coin.

Case 3:

If  $n = 20, r = 12$ , then  $P(\text{CoinFair}|\text{Data}) = 0.8077$  which is close to 0.8.

**Example (Box)**

There are two boxes:

- (i) Box  $B_1$  with 4 black balls and 1 white ball
- (ii) Box  $B_2$  with 1 black ball and 3 white balls

You pick one box at random (*prior* probability of picking any box is 0.5).

Then select a ball from the box. It turns out to be white (*data*).

Given that the ball is white, what is the probability that you picked the 1st box ?

Solution:  $P(B_1|W) = P(W|B_1)P(B_1)/P(W)$  where,  
using total probability,  $P(W) = P(W|B_1)P(B_1) + P(W|B_2)P(B_2)$

$P(B_1|W)$  comes out to 0.2105

Prior probability for  $P(B_1)$  was 0.5

**Example: Gaussian (Unknown mean, Known variance)**

Given: Data  $\{x_i\}_{i=1}^N$  derived from a Gaussian distribution with known variance  $\sigma^2$ , but unknown mean  $\mu$

*Treat mean  $\mu$  as a random variable*

Prior belief on  $\mu$  is that it is derived from a Gaussian with mean  $\mu_0$  and variance  $\sigma_0^2$

Associated Generative Model here: first draw  $\mu$  from prior, then draw data given  $\mu$ .

Goal: Estimate  $\mu$ , given prior and data

What if we ignore the prior ? (ML estimation seen before)

What if we ignore the likelihood / data ? ( $\mu = \mu_0$ )

A possible solution: Maximize posterior w.r.t.  $\mu$

Posterior:  $P(\mu|x_1, \dots, x_N) = P(x_1, \dots, x_N|\mu)P(\mu)/P(x_1, \dots, x_N)$

Assume sample mean =  $\bar{x}$

Then MAP estimate for the mean is:

$$\mu = \frac{\bar{x}\sigma_0^2 + \mu_0\sigma^2/N}{\sigma_0^2 + \sigma^2/N}$$

What if  $N = 1$  ?

What if  $N \rightarrow \infty$  ? (data dominates the prior)

What if  $\sigma_0 \rightarrow \infty$  ? (weak prior: ignore the prior)

What if  $\sigma_0 \rightarrow 0$  ? (strong prior: ignore the data)

**Posterior Mean Estimate to Minimize MSE**

Given data:  $\{x_i\}_{i=1}^n$  drawn from  $P(X|\theta)$

We have a prior  $P(\theta)$  on RV  $\theta$

Posterior = conditional density =

$$P(\theta|x_1, \dots, x_n) = \frac{P(x_1, \dots, x_n|\theta)P(\theta)}{\int_{\theta} P(x_1, \dots, x_n, \theta)d\theta}$$

Question: Given a PDF  $P(\theta|x_1, \dots, x_n)$  on the true parameter  $\theta$ , what is the best estimate  $\hat{\theta}^*$  to minimize mean squared error  $E_{P(\theta|x_1, \dots, x_n)}[(\hat{\theta} - \theta)^2]$ ?

Answer: The PDF mean  $E_{P(\theta|x_1, \dots, x_n)}[\theta]$ . This is also a Bayes estimate.

### Loss functions and Risk functions

Loss function  $L(\hat{\theta}|\theta) :=$  loss incurred in obtaining the estimate as  $\hat{\theta}$ , when the true value was  $\theta$ .

We know that, given the data, the true value  $\theta$  is distributed as per the posterior PDF  $P(\theta|x_1, \dots, x_n)$

Risk function  $R(\hat{\theta}) :=$  expected loss  $:=$  expectation of the loss function  $L(\hat{\theta}|\theta)$  under the posterior PDF  $P(\theta|x_1, \dots, x_n)$

Goal: Choose  $\hat{\theta}$  to minimize risk

Example: Squared-error loss function:  $L(\hat{\theta}) = (\hat{\theta} - \theta)^2$

Risk function  $= E_{P(\theta|x_1, \dots, x_n)}[(\hat{\theta} - \theta)^2] =$  mean squared error

Let risk minimizer  $= \theta^*$

Then,  $\frac{\partial}{\partial \hat{\theta}} E_{P(\theta|x_1, \dots, x_n)}[(\hat{\theta} - \theta)^2] \Big|_{\hat{\theta}=\theta^*} = 0$

Thus,  $\theta^* = E_{P(\theta|x_1, \dots, x_n)}[\theta] =$  Posterior mean

Example: Zero-one loss function (case of discrete RV  $\theta$ ):  $L(\hat{\theta}) = I(\hat{\theta} \neq \theta)$

Risk function  $= R(\hat{\theta}) = E_{P(\theta|x_1, \dots, x_n)}[I(\hat{\theta} \neq \theta)]$

$$= \sum_{\theta \neq \hat{\theta}} P(\theta|x_1, \dots, x_n)$$

$$= 1 - P(\theta = \hat{\theta}|x_1, \dots, x_n)$$

Thus, the risk function is minimized when  $\hat{\theta} = \arg \max_{\theta} P(\theta|x_1, \dots, x_n) =$  MAP estimate

Example: Zero-one loss function (case of continuous RV  $\theta$ )

Assume that the loss function is an *inverted* rectangular pulse —\_— with height 1 and an infinitesimally small width  $\epsilon > 0$  (we do NOT make  $\epsilon = 0$ ), with center of the pulse at the true parameter value  $\theta$ . i.e.,

$L(\hat{\theta}|\theta) = 0$ ; if  $\hat{\theta} \in (\theta - \epsilon/2, \theta + \epsilon/2)$

$L(\hat{\theta}|\theta) = 1$ ; otherwise

For such a loss function, the risk function  $1 - \int_{\hat{\theta}-\epsilon/2}^{\hat{\theta}+\epsilon/2} P(\theta|x_1, \dots, x_n) d\theta$  is minimized when the pulse center is placed at the mode of the PDF.

Take the limit, as  $\epsilon \rightarrow 0$ , of  $\arg \max_{\hat{\theta}} \int_{\hat{\theta}-\epsilon/2}^{\hat{\theta}+\epsilon/2} P(\theta|x_1, \dots, x_n) d\theta$

Consider a bimodal PDF: One peak is wide. Another peak is narrow.

Example: Absolute-error loss function  $L(\hat{\theta}) = |\hat{\theta} - \theta|$

Risk function  $= E_{P(\theta|x)}[|\hat{\theta} - \theta|]$

$$= \int_{-\infty}^{\infty} |\hat{\theta} - \theta| P(\theta|x) d\theta$$

$$= \int_{-\infty}^{\hat{\theta}} (\hat{\theta} - \theta) P(\theta|x) d\theta + \int_{\hat{\theta}}^{\infty} (\theta - \hat{\theta}) P(\theta|x) d\theta$$

The risk function is minimized when its derivative is zero.

How to take the derivative of an integral where the limits are also a function of the variable of interest ?

Leibniz's Integral Rule:

$$\frac{\partial}{\partial a} \int_{l(a)}^{u(a)} f(z, a) dz = \int_{l(a)}^{u(a)} \frac{\partial f}{\partial a} dz + f(z = u(a), a) \frac{\partial u}{\partial a} - f(z = l(a), a) \frac{\partial l}{\partial a}$$

In our case,  $f(z \equiv \theta, a \equiv \hat{\theta}) \propto (\hat{\theta} - \theta) P(\theta|x)$

In our case, for the 1st integral:  $f(z = u(a), a) = 0$  and the lower-limit term doesn't arise

In our case, for the 2nd integral:  $f(z = l(a), a) = 0$  and the upper-limit term doesn't arise

Thus, the derivative of our risk function w.r.t.  $\hat{\theta}$  is:

$$= \int_{-\infty}^{\hat{\theta}} (+1) P(\theta|x) d\theta + \int_{\hat{\theta}}^{\infty} (-1) P(\theta|x) d\theta$$

$$= \int_{-\infty}^{\hat{\theta}} P(\theta|x) d\theta - \int_{\hat{\theta}}^{\infty} P(\theta|x) d\theta$$

This is zero when  $\hat{\theta} = \text{median of } P(\theta|x)$

The median will be a minimizer if the 2nd derivative is positive. Is that so ?

In this case, for both integrals,  $\frac{\partial f}{\partial a} = 0$

In this case, for 1st integral, the lower-limit term doesn't arise

In this case, for 2nd integral, the upper-limit term doesn't arise

Thus, the 2nd derivative of our risk function w.r.t.  $\hat{\theta}$ , evaluated at  $\hat{\theta} = \text{median of } P(\theta|x)$ , is:

$$= P(\hat{\theta}|x) + P(\hat{\theta}|x) \geq 0$$

*Note: the median  $\hat{\theta}$  isn't unique if  $P(\hat{\theta}|x) = 0$*

### Example: i.i.d. Bernoulli

Given:  $X_1, \dots, X_n$  are i.i.d. Bernoulli with parameter  $\theta$  and PDF  $P(x = 1|\theta) = \theta, P(x = 0|\theta) = 1 - \theta$

Data:  $x_1, \dots, x_n$

Estimate  $\theta \in (0, 1)$

Prior  $P(\theta) = 1, \forall \theta \in (0, 1)$

Answer:

Rewrite PDF as  $P(x|\theta) = \theta^x (1 - \theta)^{1-x}$ , where  $x \in \{0, 1\}$

$$P(\theta|x_1, \dots, x_n) = P(x_1, \dots, x_n|\theta) / P(x_1, \dots, x_n)$$

where Numerator  $= \theta^{\sum_i x_i} (1 - \theta)^{n - \sum_i x_i}$

If we want the posterior mean, then we need to care about the denominator as well

Denominator

$$= \int_0^1 \theta^{\sum_i x_i} (1 - \theta)^{n - \sum_i x_i} d\theta$$

To handle the integral in the denominator, we use the result / trick:

$$\int_0^1 \theta^m (1 - \theta)^r d\theta = m!r!/(m + r + 1)!$$

Let  $x = \sum_i x_i$

Then,  $P(\theta|x_1, \dots, x_n) = \frac{(n+1)!}{x!(n-x)!} \theta^x (1 - \theta)^{n-x}$

Thus,  $E_{P(\theta|x_1, \dots, x_n)}[\theta] = \int_0^1 \theta \frac{(n+1)!}{x!(n-x)!} \theta^x (1 - \theta)^{n-x} d\theta = \frac{x+1}{n+2}$

Thus, Bayes posterior-mean estimator  $= \frac{\sum_i X_i + 1}{n+2}$

Note: ML estimator  $= \max_{\theta} \log (\theta^{\sum_i X_i} (1 - \theta)^{n - \sum_i X_i})$   
 $= \max_{\theta} X \log \theta + (n - X) \log(1 - \theta)$ , where  $X := \sum_i X_i$   
 $= X/n$   
 $= \sum_i X_i / n$

Check that the 2nd derivative is negative (Use the facts:  $X \geq 0$  and  $n - X \geq 0$  and  $0 < \theta < 1$ )

Note: In this case, ML estimator  $\equiv$  MAP estimator; because  $P(\theta) = 1$

Note: When  $n = 0$ , Bayes estimate  $= 0.5$ , the mid-point of the interval  $(0, 1)$ . This is what we get when we solely rely on the prior

Note: Asymptotically, i.e., as  $n \rightarrow \infty$ , the Bayes (mean) estimator tends to the ML estimator

What happens to the Bayes estimate and ML estimate when true  $\theta = 0$  or true  $\theta = 1$  ? Assume  $n$  is large.

### Example: i.i.d. Gaussian

Given:  $X_1, \dots, X_n$  i.i.d.  $G(\theta, \sigma_0^2)$ . Unknown mean. Known variance.

Prior:  $P(\theta) := G(\theta; \mu; \sigma^2)$

Bayes posterior-mean estimate = ?

Answer:

Property 1: Product of 2 Gaussians is another Gaussian:  $G(z; \mu_1, \sigma_1^2)G(z; \mu_2, \sigma_2^2) \propto G(z; \mu_3, \sigma_3^2)$

$$\begin{aligned} \text{Numerator exponent} &= \frac{(z - \mu_1)^2}{2\sigma_1^2} + \frac{(z - \mu_2)^2}{2\sigma_2^2} \\ &= \frac{1}{2\sigma_1^2\sigma_2^2} (z^2(\sigma_2^2 + \sigma_1^2) - (2\mu_1\sigma_2^2 + 2\mu_2\sigma_1^2)z + \mu_1^2\sigma_2^2 + \mu_2^2\sigma_1^2) \\ &= \frac{1}{2\sigma_1^2\sigma_2^2} (z^2(\sigma_2^2 + \sigma_1^2) - (2\mu_1\sigma_2^2 + 2\mu_2\sigma_1^2)z) + c, \end{aligned}$$

where  $c = \text{constant independent of } z$

$$\begin{aligned} &= \frac{\sigma_2^2 + \sigma_1^2}{2\sigma_1^2\sigma_2^2} \left( z^2 - \frac{2\mu_1\sigma_2^2 + 2\mu_2\sigma_1^2}{\sigma_2^2 + \sigma_1^2} z \right) + c, \\ &= \frac{\sigma_2^2 + \sigma_1^2}{2\sigma_1^2\sigma_2^2} (z^2 - 2\mu_3 z + \mu_3^2) + c' = \frac{1}{2\sigma_3^2} (z - \mu_3)^2 + c', \end{aligned}$$

where  $c' = \text{constant independent of } z \text{ and}$

$$\mu_3 = \frac{\mu_1\sigma_2^2 + \mu_2\sigma_1^2}{\sigma_1^2 + \sigma_2^2}, \sigma_3^2 = \frac{\sigma_1^2\sigma_2^2}{\sigma_1^2 + \sigma_2^2}$$

In our case, we have two PDFs on  $\theta$ , i.e.,

$$\text{Prior } P(\theta) = \frac{1}{\sigma\sqrt{2\pi}} \exp((\theta - \mu)^2/(2\sigma^2)) = G(\theta; \mu, \sigma^2)$$

$$\text{Likelihood } P(x_1, \dots, x_n|\theta) = \frac{1}{(2\pi)^{n/2}\sigma_0^n} \exp(-\sum_i (x_i - \theta)^2/(2\sigma_0^2)) = G(\theta; x_1, \sigma_0^2) \cdots G(\theta; x_n, \sigma_0^2)$$

The negative exponent here can be written as:

$$\begin{aligned} & (n\theta^2 - 2(\sum_i x_i)\theta)/(2\sigma_0^2) + c, \text{ where } c = \text{constant independent of } \theta \\ & = (\theta^2 - 2(\sum_i x_i/n)\theta)/(2\sigma_0^2/n) + c \\ & \propto G(\theta; \sum_i x_i/n, \sigma_0^2/n) \end{aligned}$$

$$\text{Let } x = \sum_i x_i/n$$

Thus, the (normalized) product of the prior and the likelihood gives a Gaussian  $G(\theta; \mu^*, \sigma^{*2})$ , where

$$\mu^* = \frac{\mu\sigma_0^2/n + x\sigma^2}{\sigma^2 + \sigma_0^2/n}, \sigma^{*2} = \frac{\sigma^2\sigma_0^2/n}{\sigma^2 + \sigma_0^2/n}$$

Bayes (mean) estimate = mean of posterior =  $\mu^*$ , which is also the Gaussian posterior's mode = MAP estimate

Note: As the data sample size  $n \rightarrow \infty$ , the mean  $\mu^* \rightarrow x$  and variance  $\sigma^{*2} \rightarrow 0$ .

Thus, the posterior becomes a delta function at  $\theta = x = \text{sample mean}$

In this case, the Bayes estimate converges to the ML estimate = sample mean

## MAP Estimation and ML Estimation

Consider the likelihood function  $P(x_1, \dots, x_n|\theta)$

Consider prior  $P(\theta) = 1/(b-a)$  for  $\theta \in (a, b)$ , i.e., a uniform distribution over  $(a, b)$

Then, for  $\theta \in (a, b)$ , posterior PDF =

$$\frac{P(x_1, \dots, x_n|\theta)P(\theta)}{\int_a^b P(x_1, \dots, x_n|\theta)P(\theta)d\theta} = \frac{P(x_1, \dots, x_n|\theta)}{\int_a^b P(x_1, \dots, x_n|\theta)d\theta}$$

Maximum of the posterior within  $(a, b) = \text{maximum of } P(x_1, \dots, x_n|\theta) \text{ within } (a, b)$

If the mode of the likelihood function lied within  $(a, b)$ , then the mode of the posterior  $\equiv$  ML estimate

## Bayes Interval Estimate

Previous analysis gives a point estimate for the parameter  $\theta$

How do we get an interval estimate for the parameter  $\theta$  ?

We can do this by finding  $a, b$  such that  $\int_a^b P(\theta|x_1, \dots, x_n)d\theta = 1 - \alpha$ , where probability  $\alpha$  is given.

We can get such information in some special cases, relatively easily

**Example: Gaussian**

Question: Suppose signal of value  $s$  is sent from A to B.

Because of the noisy communication channel, signal received at B has a Gaussian PDF with mean  $s$  and variance 60.

*A priori*, it is known that the signal  $s$  being sent is selected from a Gaussian PDF with mean 50 and variance 100.

Value received at B is 40.

Find an interval  $(a, b)$  s.t. the probability of the signal being in that interval is 0.9

Answer:

Using formulas derived before for the posterior  $P(s|x_1 = 40)$  of parameter  $s$  given data  $x_1$ ,

$$\text{Posterior mean} = \frac{50 \cdot 60 + 40 \cdot 100}{60 + 100} = 43.75$$

$$\text{Posterior variance} = \frac{60 \cdot 100}{60 + 100} = 37.5$$

We know that the posterior PDF is Gaussian

Thus,  $Z := \frac{S - 43.75}{\sqrt{37.5}}$  has a standard Normal PDF

For a standard Normal PDF, we know that the probability mass within  $Z \in (-1.645, +1.645)$  is 0.9

Thus, we want to find  $S$  s.t.  $P(-1.645 < Z < 1.645 | \text{data}) = 0.9$

$$\text{i.e., } P(-1.645 < \frac{S - 43.75}{\sqrt{37.5}} < 1.645 | \text{data}) = 0.9$$

$$\text{i.e., } P(33.68 < S < 53.83 | \text{data}) = 0.9$$

Thus, the desired interval is  $(a = 33.68, b = 53.83)$

**Conjugate Priors**

If the posterior PDFs  $P(\theta|x)$  are in the same family as the prior PDF  $P(\theta)$ , then:

- (i) the prior and posterior are called *conjugate* PDFs, and
- (ii) the prior is called the conjugate prior for the likelihood function

Advantage of conjugate priors: When the prior gives closed-form analytical expressions, then the posterior also gives closed-form analytical expressions, and its denominator / normalizing constant has a closed-form expression

$$P(\theta|x) = \frac{P(x|\theta)P(\theta)}{\int P(x|\theta)P(\theta)d\theta}$$

Otherwise, a difficult numerical integration may be required to approximate the normalizing factor

**Example: Binomial Likelihood and Beta prior**

1) Likelihood of  $s$  successes in  $n$  tries:  $P(s, n|\theta) = {}^nC_s \theta^s (1 - \theta)^{n-s}$ , where  $n \in \mathbb{N}$ ,  $s \in \mathbb{I}_{\geq 0}$

2) Prior:  $P(\theta) = \text{beta}(\theta; a \in \mathbb{R}^+, b \in \mathbb{R}^+) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{a-1} (1 - \theta)^{b-1}$ , Note:  $a > 0, b > 0$

3) Posterior  $\propto \theta^{s+a-1} (1 - \theta)^{n-s+b-1} \equiv \text{beta}(\theta; a + s, b + n - s)$

- We know that the **mean** of the beta PDF  $\text{beta}(\theta; a, b)$  is  $a/(a + b)$

Thus, Bayes (mean) estimate = posterior mean =  $(a + s)/(a + b + n)$

=  $w(a/(a + b)) + (1 - w)(s/n)$ , where weight  $w = (a + b)/(a + b + n)$

Note: When the sample size  $n = 0$ , the posterior mean =  $a/(a + b)$  = prior mean

Note: As the sample size  $n \rightarrow \infty$ , the weight  $w \rightarrow 0$  and the posterior mean  $\rightarrow$  ML estimate

If prior  $P(\theta) = 1$  is uniform over  $\theta \in (0, 1)$ , i.e.,  $\text{beta}(\theta, 1, 1)$

In that case, the likelihood determines the posterior

- We know that the **mode** of the beta PDF  $\text{beta}(\theta; a, b)$  is  $(a - 1)/(a + b - 2)$  for  $a, b > 1$

So, posterior mode =  $(a + s - 1)/(a + b + n - 2)$

$$= w((a-1)/(a+b-2)) + (1-w)(s/n), \text{ where weight } w = (a+b-2)/(a+b+n-2)$$

Note: When the sample size  $n = 0$ , the posterior mode  $= (a-1)/(a+b-2) = \text{prior mode}$

Note: As the sample size  $n \rightarrow \infty$ , the weight  $w \rightarrow 0$  and the posterior mode  $\rightarrow \text{ML estimate}$

Example: Gaussian (known mean  $\mu$ , unknown variance  $\theta$ ) and Inverse Gamma

1) Likelihood:  $P(x_1, \dots, x_n | \mu, \theta) \propto \prod_{i=1}^n \theta^{-0.5} \exp(-0.5(x_i - \mu)^2/\theta)$

2) Prior = Inverse Gamma PDF:  $P(\theta; a, b) \propto \theta^{-a-1} \exp(-b/\theta)$ , where  $a > 0, b > 0$

3) Posterior = Inverse Gamma PDF:  $P(\theta; a + n/2, b + \sum_i (x_i - \mu)^2/2)$

• **Mean** of the inverse Gamma  $P(\theta; a, b) = b/(a-1)$ , for  $a > 1$

Thus, Bayes estimate = posterior mean  $= (b + \sum_i (x_i - \mu)^2/2)/(a + n/2 - 1)$

$$= (2b + \sum_i (x_i - \mu)^2)/(2a + n - 2)$$

$$= w(b/(a-1)) + (1-w) \sum_i (x_i - \mu)^2/n, \text{ where weight } w = (2a-2)/(2a+n-2)$$

Note: When the sample size  $n = 0$ , the weight  $w = 1$  and the posterior mean  $= b/(a-1) = \text{prior mean}$

Note: As the sample size  $n \rightarrow \infty$ , the weight  $w \rightarrow 0$  and the posterior mean  $\rightarrow \text{ML estimate}$

• **Mode** of the inverse Gamma  $P(\theta; a, b) = b/(a+1)$

So, posterior mode  $= (b + \sum_i (x_i - \mu)^2/2)/(a + n/2 + 1)$

$$= (2b + \sum_i (x_i - \mu)^2)/(2a + n + 2)$$

$$= w(b/(a+1)) + (1-w) \sum_i (x_i - \mu)^2/n, \text{ where weight } w = (2a+2)/(2a+n+2)$$

Note: When the sample size  $n = 0$ , the weight  $w = 1$  and the posterior mode  $= b/(a+1) = \text{prior mode}$

Note: As the sample size  $n \rightarrow \infty$ , the weight  $w \rightarrow 0$  and the posterior mode  $\rightarrow \text{ML estimate}$

An “uninformative” (misnomer) prior for the Gaussian *mean* is the (improper) uniform PDF

Why improper ? Because it doesn't integrate to a finite number

Why uninformative ? Because:

i) posterior PDF driven by the likelihood function alone

ii) the prior on  $\theta$  is invariant to any change in the true  $\theta$ , which could cause translation of the data  $x_i$  (Duda-Hart-Stork).

Note: translation of data also implies that the MLE estimate of the mean also gets translated.

Uninformative priors express “objective” (impersonal; unaffected by personal beliefs) information such as “the variable is positive” or “the variable is less than some limit”.

Uninformative priors yield results *close to* what we would get with non-Bayesian (e.g., ML) analysis

An “uninformative” (and improper) prior for the Gaussian *standard deviation*  $\sigma$  is  $P(\sigma) = 1/\sigma$

Why uninformative ? Because of scale invariance, as follows.

Assume data  $x$  comes from a Gaussian with mean zero. Consider the RVs  $\log(X)$  and  $\log(\sigma)$ . If the data  $x$  get scaled (which implies that the MLE for the standard deviation  $\sigma$  also gets scaled) in the original domain by factor  $a$ , then a term  $\log(a)$  gets added in the log domain. Scale-invariant prior on  $\sigma \rightarrow$  translation-invariant prior on  $\log(\sigma) \rightarrow$  uniform PDF on  $\log(\sigma)$ .

Transform the RV  $U := \log(\sigma)$  with  $P(U) = c$ , to get the RV  $V := \exp(U)$ .



Transformation of variables implies that  $P(V = v) = c/v$ .

A uniform prior on  $\log(\sigma)$  implies a uniform prior on  $2 \log(\sigma) = \log(\sigma^2) := \log(\theta)$ , where  $\theta := \sigma^2 = \text{variance}$

The uninformative prior for the Gaussian variance  $\theta$  is the inverse Gamma PDF with parameters  $a = b \rightarrow 0$ , which implies  $P(\theta) \propto 1/\theta$ , also an improper prior

### Example: Poisson PDF and Gamma prior

Use this example to motivate the general result for exponential families later

- 1) Likelihood:  $P(k_1, \dots, k_n | \lambda) = \prod_i \lambda^{k_i} \exp(-\lambda) / k_i!$ , where  $\lambda \in \mathbb{R}^+$ ,  $k_i \in \mathbb{I}^+$
- 2) Prior:  $P(\theta) = \text{Gamma}(\lambda | \alpha, \beta) \propto \lambda^{\alpha-1} \exp(-\beta\lambda)$ , where  $\alpha \in \mathbb{R}^+$ ,  $\beta \in \mathbb{R}^+$ ,  $\lambda \in \mathbb{R}^+$
- 3) Posterior:  $\propto \lambda^{\sum_i k_i + \alpha - 1} \exp(-n\lambda - \beta\lambda) \equiv \text{Gamma}(\lambda; \sum_i k_i + \alpha, n + \beta)$

- For a Gamma distribution  $\text{Gamma}(\lambda | \alpha, \beta)$ , we know that the **mean** is  $\alpha/\beta$

Thus, the Bayes estimate = posterior mean =  $(\sum_i k_i + \alpha) / (n + \beta)$   
 $= w(\alpha/\beta) + (1 - w) \sum_i k_i / n$ , where weight  $w = \beta / (\beta + n)$   
 $= w(\alpha/\beta) + (1 - w) \hat{\lambda}_{\text{MLE}}$

Note: When the sample size  $n = 0$ , the weight  $w = 1$  and the posterior mean =  $\alpha/\beta$  = prior mean

Note: As the sample size  $n \rightarrow \infty$ , the weight  $w \rightarrow 0$  and the posterior mean  $\rightarrow$  ML estimate

- For a Gamma distribution  $\text{Gamma}(\lambda | \alpha, \beta)$ , we know that the **mode** is  $(\alpha - 1)/\beta$  when  $\alpha \geq 1$ . When  $\alpha < 1$ , the case is tricky.

Then, posterior mode =  $(\sum_i k_i + \alpha - 1) / (n + \beta)$   
 $= w((\alpha - 1)/\beta) + (1 - w) \sum_i k_i / n$ , where weight  $w = \beta / (\beta + n)$

Note: When the sample size  $n = 0$ , the weight  $w = 1$  and the posterior mode =  $(\alpha - 1)/\beta$  = prior mode

Note: As the sample size  $n \rightarrow \infty$ , the weight  $w \rightarrow 0$  and the posterior mode  $\rightarrow$  ML estimate

## Exponential Family of PDFs

PDFs in the exponential family (typically) have conjugate priors.

Definition: A **single-parameter** exponential family is a set of PDFs where each PDF can be expressed in the form:  
 $P(x|\theta) = \exp[\eta(\theta)T(x) - A(\theta) + B(x)] = g(\theta)h(x) \exp[\eta(\theta)T(x)]$ , where  $T(x), B(x), \eta(\theta), A(\theta)$  are known functions.

Interpretation: Parameters  $\theta$  and observation variables  $x$  must *factorize* either directly or within an exponential operation

The support of the distribution cannot depend on  $\theta$ .

Continuous case:  $P(x \in A|\theta) > 0$  if and only if  $\int_{x \in A} h(x)dx > 0$ .

Discrete case:  $P(x \in A|\theta) > 0$  if and only if  $A \cap \{x : h(x) > 0\} \neq \emptyset$ .

So, uniform PDF and Pareto PDF aren't in this family.

Neither is Cauchy PDF, Laplace PDF, Student's t PDF, mixture PDF.

Consider the *canonical form* of the exponential family where  $\eta(\theta) := \theta$ , i.e.,  $\eta(\cdot)$  is identity

It is always possible to convert an exponential family to canonical form, by defining a transformed parameter  $\theta' = \eta(\theta)$

### Example: Bernoulli

$$P(X = x; \theta) = \theta^x (1 - \theta)^{1-x} = \exp(x \log \theta + (1 - x) \log(1 - \theta)) = \exp(x \log(\theta/(1 - \theta)) + \log(1 - \theta))$$

$$\eta = \log(\theta/(1 - \theta))$$

$$T(x) = x$$

$$g(\eta) = \exp(\log(1 - \theta)) = (1 - \theta)$$

$$h(x) = 1$$

### Example: Poisson

$$P(X = x; \lambda) = \lambda^x \exp(-\lambda)/(x!) = \exp(-\lambda)(1/x!) \exp[x \log \lambda]$$

$$\eta = \log \lambda$$

$$T(x) = x$$

$$g(\eta) = \exp(-\lambda)$$

$$h(x) = 1/x!$$

Definition: A **multi-parameter** exponential family is a set of PDFs where each PDF can be expressed in the form:

$P(x|\eta) = \exp[\eta^\top T(x) - A(\eta) + B(x)]$ , where  $T(x), B(x), A(\eta)$  are known functions.

### Example: Gaussian

$$P(X = x; \mu, \sigma^2) = (1/\sigma)(1/\sqrt{2\pi}) \exp(-0.5x^2/\sigma^2 + \mu x/\sigma^2 - 0.5\mu^2/\sigma^2)$$

$$\eta = [-0.5/\sigma^2, \mu/\sigma^2]^\top$$

$$T(x) = [x^2, x]^\top$$

$$g(\eta) = (1/\sigma) \exp(-0.5\mu^2/\sigma^2)$$

$$h(x) = (1/\sqrt{2\pi})$$

### Some Properties:

(1) The random variable  $T(X)$  is sufficient for parameter  $\theta$

$T(X)$  is a function of data only; not any parameter.

### Sufficient Statistic:

Statistic  $T(X)$  is sufficient for parameter  $\theta$  if there isn't any information in data  $X$  regarding  $\theta$  beyond that in  $T(X)$ . If our goal is to estimate  $\theta$ , all we need is  $T(X)$  and  $X$  can be discarded.

(2) If i.i.d. RVs  $\{X_i\}$  are from the one-parameter exponential family, then their joint PDF is also from the one-parameter exponential family (with sufficient statistic  $\sum_i T(X_i)$ ).

The joint PDF is  $P(x_1, x_2, \dots, x_N | \theta) = \left( \prod_{n=1}^N h(x_n) \right) \exp \left( \eta^\top \sum_{n=1}^N T(x_n) - NA(\eta) \right)$

For i.i.d. observations from (i) Bernoulli PMF or (ii) Poisson PDF, sufficient statistic for parameter is the sum  $\sum_n x_n$

For i.i.d. observations from (i) Gaussian PDF, sufficient statistic for parameter is the vector of sums  $[\sum_n x_n^2, \sum_n x_n]$

What other PDFs aren't in the exponential family ?

Uniform, Pareto.

$$P(x|\theta) = [f(x)g(\theta)]^{h(x)j(\theta)} = \exp([h(x)\log f(x)]j(\theta) + h(x)[j(\theta)\log g(\theta)])$$

Laplace / Double-Exponential PDF:  $P(x|\theta) := 0.5 \exp(-|x - \theta|)$

Cauchy PDF:  $P(x|\theta) := 1/(\pi(1 + (x - \theta)^2))$

—

For the univariate case, we have:  $P(x|\theta) = h(x) \exp[\eta(\theta)T(x) - A(\theta)]$

Let  $\phi(x, \theta) := \eta(\theta)T(x) - A(\theta)$

Then, for any 4 observations  $x_1, x_2, x_3, x_4$ , the ratio

$$\frac{\phi(x_1, \theta) - \phi(x_2, \theta)}{\phi(x_3, \theta) - \phi(x_4, \theta)}$$

doesn't depend on  $\theta$ .

—

• How do we go about guessing what the conjugate prior is ?

Step (1) For the exponential family, the likelihood function for data  $\{x_i\}_{i=1}^N$  is:

$$L(\theta|x_1, \dots, x_N) = (\prod_i \exp(B(x_i))) \exp(\theta (\sum_i T(x_i)) - NA(\theta))$$

Step (2) Consider the prior  $P(\theta|\alpha, \beta) = H(\alpha, \beta) \exp(\alpha\theta - \beta A(\theta))$

Diaconis and Ylvisaker 1979 gave conditions on the hyper-parameters  $\alpha, \beta$  under which this PDF is integrable (i.e., proper)

Step (3) The posterior PDF  $\propto \exp(\theta(\alpha + \sum_i T(x_i)) - (\beta + N)A(\theta))$  that belongs to the exponential family w.r.t. variable  $\theta$  and has the same form as the prior

The conversion from the prior to the posterior simply replaces  $\alpha \rightarrow \alpha + \sum_i T(x_i)$  and  $\beta \rightarrow \beta + N$

Because the prior can be normalized, so can the posterior

## Kullback-Leibler Divergence / Dissimilarity

Continuous RVs:  $D(P(X|\theta_1), Q(X|\theta_2)) := \int_x P(x|\theta_1) \log \frac{P(x|\theta_1)}{Q(x|\theta_2)} dx$

Discrete RVs:  $D(P(X|\theta_1), Q(X|\theta_2)) := \sum_x P(x|\theta_1) \log \frac{P(x|\theta_1)}{Q(x|\theta_2)}$

Finite only under the following condition:  $Q(x) = 0$  on a measurable set implies  $P(x) = 0$  on that set

When  $P(x) \rightarrow 0$  and  $Q(x) > 0$ , the contribution of the  $x$ -th term is zero because  $\lim_{P(x) \rightarrow 0} P(x) \log P(x) = 0$

When  $P(x) \rightarrow 0$  and  $Q(x) \rightarrow 0$ , we use the convention / *interpretation* that  $0 \log \frac{0}{0} = 0$ ; Cover and Thomas (2nd Ed.). Basically, ignore such cases. Can see this as an outcome of regularization: (i) Bayesian prior or (ii) convex combination of each of the given PDFs  $P(X)$  and  $Q(X)$  with uniform PDF  $U(X)$ .

Properties:

- 1) When PMFs / PDFs  $P(X)$  and  $Q(X)$  are identical (almost everywhere; in the continuous case), then  $D(P, Q) = 0$
- 2)  $D(P, Q) \geq 0$ , for all  $P, Q$

For discrete PMFs, this inequality is known as the Gibbs' inequality

Proof (discrete case):

We know that  $\log x \leq x - 1$

So,  $-\log x \geq -(x - 1)$

$$\begin{aligned} & \sum_{x|P(x)>0} P(x) \log \frac{P(x)}{Q(x)} \\ &= - \sum_{x|P(x)>0} P(x) \log \frac{Q(x)}{P(x)} \\ &\geq - \sum_{x|P(x)>0} P(x) \left( \frac{Q(x)}{P(x)} - 1 \right) \\ &= - \sum_{x|P(x)>0} Q(x) + \sum_{x|P(x)>0} P(x) \\ &= - \sum_{x|P(x)>0} Q(x) + 1 \\ &\geq 0 \end{aligned}$$

So,  $\sum_{x|P(x)>0} P(x) \log P(x) \geq \sum_{x|P(x)>0} P(x) \log Q(x)$

If we extend the summation to all remaining  $x'$ , then the LHS stays the same (because  $\lim_{P(x') \rightarrow 0} P(x') \log P(x') = 0$ ) and the RHS also stays the same (because  $P(x') = 0$ )

Thus,  $\sum_x P(x) \log P(x) \geq \sum_x P(x) \log Q(x)$

Thus,  $D(P||Q) \geq 0$

When is  $D(P||Q) = 0$  ?

For this to happen:

Condition 1:  $P(x) = Q(x), \forall x : P(x) > 0$ , i.e., when  $\log \frac{P(x)}{Q(x)} = 0 = \frac{P(x)}{Q(x)} - 1$  making the first inequality an equality

Condition 2: The second inequality becomes an equality when  $\sum_{x:P(x)>0} Q(x) = 1$

Alternatively, because  $\sum_{x:P(x)>0} P(x) = 1$ , and  $P(x) = Q(x)$  on this domain, we have  $\sum_{x:P(x)>0} Q(x)$  also = 1

Thus, for all  $x : P(x) = 0$ , we also have  $Q(x) = 0$

Thus,  $P(x) = Q(x), \forall x$

For continuous PMFs, the proof uses Jensen's inequality.

Jensen's inequality: If  $f(\cdot)$  is a convex function and  $X$  is a random variable, then  $E[f(X)] \geq f(E[X])$

Proof of Jensen's inequality:

Let  $\mu := E[X]$

Draw a line tangent to the convex function  $f(X)$ , touching it at  $(\mu, f(\mu))$

The tangent, say,  $aX + b$  lies below the function  $f(X)$ ,  $\forall X$

LHS =  $E[f(X)] \geq E[aX + b] = a\mu + b = f(\mu) = \text{RHS}$

Another variant of Jensen's Inequality:

$E_{P(X)}[f(g(X))] \geq f(E_{P(X)}[g(X)])$ , when  $f(\cdot)$  is convex and  $g(\cdot)$  can be any function.

Proved.

Proved: KL Divergence being non-negative (continuous case).

KL-Divergence Property:  $D(\cdot, \cdot)$  is asymmetric. Not a “distance metric”.

## KL Divergence and MLE

Empirical Estimate of PMF / PDF of data:  $\hat{P}(X = x) := (1/N) \sum_{n=1}^N \delta(x; x_n)$

Discrete RV:  $\delta(x; x_n)$  is the Kronecker delta function

Continuous RV:  $\delta(x; x_n)$  is the Dirac delta functional

For Discrete RV, KL divergence between empirical PDF and actual PDF:

$$\begin{aligned} D(\hat{P}(X), P(X|\theta)) &= \sum_x \hat{P}(x) \log \hat{P}(x) - \sum_x \hat{P}(x) \log P(x|\theta) \\ &= \sum_x \hat{P}(x) \log \hat{P}(x) - \sum_x (1/N) \sum_n \delta(x; x_n) \log P(x|\theta) \\ &= \sum_x \hat{P}(x) \log \hat{P}(x) - (1/N) \sum_n \sum_x \delta(x; x_n) \log P(x|\theta) \\ &= \sum_x \hat{P}(x) \log \hat{P}(x) - (1/N) \sum_n \log P(x_n|\theta) \end{aligned}$$

where the second term is the average log-likelihood function

Thus, minimizing this KL divergence is the same as maximizing the likelihood function

For Continuous RV, KL divergence between empirical PDF and actual PDF:

$$\begin{aligned} D(\hat{P}(X), P(X|\theta)) &= \int_x \hat{P}(x) \log \hat{P}(x) dx - \int_x \hat{P}(x) \log P(x|\theta) dx \\ &= \int_x \hat{P}(x) \log \hat{P}(x) - \int_x (1/N) \sum_n \delta(x; x_n) \log P(x|\theta) dx \\ &= \int_x \hat{P}(x) \log \hat{P}(x) - (1/N) \sum_n \int_x \delta(x; x_n) \log P(x|\theta) dx \\ &= \int_x \hat{P}(x) \log \hat{P}(x) - (1/N) \sum_n \log P(x_n|\theta) \end{aligned}$$

where the second term is the average log-likelihood function

Thus, minimizing this KL divergence is the same as maximizing the likelihood function

## Fisher Information

Key Question: How much information can a sample of data provide about the unknown parameter ?

(1) If likelihood function  $P(\text{data}|\theta)$  is sharply peaked w.r.t.  $\Delta$  changes in  $\theta$  around  $\theta = \theta_{\text{true}}$ , it is easy to estimate  $\theta_{\text{true}}$  from the given data sample of size  $N$ .

Example 1: Bernoulli RV with  $\theta$  close (equal) to 0 or 1

Example 2: Estimating Gaussian mean  $\theta := \mu$  in two cases: (i) when variance  $\sigma^2$  (known) is huge, (ii) when  $\sigma^2$  is tiny.

Data drawn from  $G(x; \mu, \sigma^2)$  in 2nd case has a smaller spread.

Likelihood in 2nd case more peaked.

For a small sample of size  $N$  (say,  $N = 5$ ), mean estimate (sample mean; always unbiased = always high accuracy) is much more precise (= much lower variance) in 2nd case

(2) If likelihood function  $P(\text{data}|\theta)$  has a large spread w.r.t. changes in  $\theta$  around  $\theta_{\text{true}}$ , it will take very many  $N$ -sized data samples to get the ML estimate of  $\theta$  to be at / close to  $\theta_{\text{true}}$

First, consider the average (expected) derivative of the log-likelihood function:

$$\begin{aligned}
& E_{P(X|\theta_{\text{true}})} \left[ \frac{\partial}{\partial \theta} \log P(X|\theta) \Big|_{\theta=\theta_{\text{true}}} \right] \\
&= \int_x P(x|\theta) \frac{\partial P(x|\theta)}{\partial \theta} / P(x|\theta) dx \\
&= \int_x \frac{\partial}{\partial \theta} P(x|\theta) dx \\
&= \frac{\partial}{\partial \theta} \int_x P(x|\theta) dx \\
&= \frac{\partial}{\partial \theta} 1 \\
&= 0
\end{aligned}$$

The expectation / integral isn't over  $\theta$ , but over different instances of observed data  $x \sim P(X|\theta_{\text{true}})$

The expectation is zero for all  $\theta_{\text{true}}$

Now, consider the expected squared slope (slope variance) of the log-likelihood function  $\log P(X|\theta)$ , evaluated at  $\theta = \theta_{\text{true}}$ , i.e.,

$$I(\theta_{\text{true}}) := E_{P(X|\theta_{\text{true}})} \left[ \left( \frac{\partial}{\partial \theta} \log P(X|\theta) \Big|_{\theta_{\text{true}}} \right)^2 \right]$$

The Fisher information  $I(\theta_{\text{true}}) \geq 0$

If  $\log P(X|\theta)$  didn't contain  $\theta$ , then the derivative would be 0, and the data wouldn't contain any information about  $\theta$

There is another way to look at Fisher information.

$$\text{Consider } \frac{\partial^2}{\partial \theta^2} \log P(X|\theta) = \frac{\frac{\partial^2 P(X|\theta)}{\partial \theta^2}}{P(X|\theta)} - \left( \frac{\frac{\partial P(X|\theta)}{\partial \theta}}{P(X|\theta)} \right)^2 = \frac{\frac{\partial^2 P(X|\theta)}{\partial \theta^2}}{P(X|\theta)} - \left( \frac{\partial \log P(X|\theta)}{\partial \theta} \right)^2 \quad (1)$$

Now, (i) evaluate LHS and RHS at  $\theta := \theta_{\text{true}}$  and (ii) take expectation w.r.t.  $P(X|\theta_{\text{true}})$ :

$$E_{P(X|\theta_{\text{true}})} \left[ \frac{\partial^2}{\partial \theta^2} \log P(X|\theta) \Big|_{\theta=\theta_{\text{true}}} \right] = E_{P(X|\theta_{\text{true}})} \left[ \frac{\frac{\partial^2 P(X|\theta)}{\partial \theta^2}}{P(X|\theta)} \Big|_{\theta=\theta_{\text{true}}} \right] - I(\theta) = -I(\theta), \text{ because} \quad (2)$$

$$E_{P(X|\theta_{\text{true}})} \left[ \frac{\frac{\partial^2 P(X|\theta)}{\partial \theta^2}}{P(X|\theta)} \Big|_{\theta=\theta_{\text{true}}} \right] = \int_x \frac{\partial^2 P(x|\theta)}{\partial \theta^2} dx = \frac{\partial^2}{\partial \theta^2} \int_x P(X|\theta) dx = 0 \quad (3)$$

So, Fisher information is the expectation (over  $x \sim P(X|\theta_{\text{true}})$ ) of the negative 2nd-derivative (curvature) of the log-likelihood function  $\log P(x|\theta)$  evaluated at  $\theta = \theta_{\text{true}}$

So, larger Fisher information means the log-likelihood function  $\log P(x|\theta)$  is expected to be more concave and more curved at  $\theta = \theta_{\text{true}}$

### Example: Bernoulli RV

$$\begin{aligned}
\log P(x|\theta) &= x \log \theta + (1-x) \log(1-\theta) \\
\frac{\partial}{\partial \theta} \log P(x|\theta) &= x/\theta - (1-x)/(1-\theta) \\
\frac{\partial^2}{\partial \theta^2} \log P(x|\theta) &= -x/\theta^2 - (1-x)/(1-\theta)^2 \\
I(\theta) &= -E \left[ \frac{\partial^2}{\partial \theta^2} \log P(x|\theta) \right] = \theta/\theta^2 + (1-\theta)/(1-\theta)^2 = 1/(\theta(1-\theta)) \\
\text{So, } I(\theta) &\text{ is large when } \theta \text{ close to 0 or 1}
\end{aligned}$$

For a dataset of size  $N$ ,  $I_N(\theta) = N/(\theta(1-\theta))$

### Example: Gaussian RV

Unknown mean parameter  $\theta = \mu$ . Known variance  $\sigma^2$ .

$$\begin{aligned}
\frac{\partial}{\partial \mu} \log P(x|\mu) &= (x-\mu)/\sigma^2 \\
\frac{\partial^2}{\partial \mu^2} \log P(x|\mu) &= -1/\sigma^2 \\
I(\mu) &= 1/\sigma^2
\end{aligned}$$

Here,  $I(\mu)$  is independent of  $\mu$ , but rather depends on the other parameter  $\sigma^2$

For a dataset of size  $N$ ,  $I_N(\mu) = N/\sigma^2$

## Cramer-Rao Lower Bound

Let RV  $X$  model a dataset.

Assumption: Consider an **unbiased** estimator  $\hat{\theta}(X)$

Then,  $E_{P(X|\theta_{\text{true}})}[\hat{\theta}(X) - \theta_{\text{true}}] = 0 = \left( \int_x P(x|\theta)[\hat{\theta}(x) - \theta]dx \right) \Big|_{\theta=\theta_{\text{true}}}$

This holds for all  $\theta_{\text{true}}$ .

That is,  $\int_x P(x|\theta')[\hat{\theta}(x) - \theta']dx$  is a function of  $\theta'$  that is identically zero. So, its derivative is also identically zero.

Thus,  $0 = \frac{\partial}{\partial \theta} \left( \int_x P(x|\theta)[\hat{\theta}(x) - \theta]dx \right) \Big|_{\theta=\theta_{\text{true}}}$

For convenience, lets call  $\theta_{\text{true}}$  as  $\theta$

Thus,  $\int_x [\hat{\theta}(x) - \theta] \frac{\partial}{\partial \theta} P(x|\theta)dx = \int_x P(x|\theta)dx = 1$

Thus,  $1 = \int_x [\hat{\theta}(x) - \theta] P(x|\theta) \frac{\partial}{\partial \theta} \log P(x|\theta)dx$

Thus,  $1 = \int_x \left( [\hat{\theta}(x) - \theta] \sqrt{P(x|\theta)} \right) \left( \sqrt{P(x|\theta)} \frac{\partial}{\partial \theta} \log P(x|\theta) \right) dx$

Thus,  $1 = \left[ \int_x \left( [\hat{\theta}(x) - \theta] \sqrt{P(x|\theta)} \right) \left( \sqrt{P(x|\theta)} \frac{\partial}{\partial \theta} \log P(x|\theta) \right) dx \right]^2$

Using Cauchy-Schwarz inequality,  $1 \leq \int_x [\hat{\theta}(x) - \theta]^2 P(x|\theta)dx \cdot \int_x P(x|\theta) \left( \frac{\partial}{\partial \theta} \log P(x|\theta) \right)^2 dx$

Thus,  $\text{Var}(\hat{\theta}(X)) \geq I(\theta)^{-1}$

For i.i.d. Gaussian RVs, any estimator of the unknown mean (known variance) will have variance  $\geq \sigma^2/n$ .

We know that the ML estimator's variance =  $\sigma^2/n$ .

Thus, this ML estimator is an *efficient* estimator / *minimum variance unbiased estimator*.

Bayesian estimation can lead to lower mean squared error, for finite data, at the cost of introducing a bias in the estimator (vis-a-vis unbiased ML estimator).

Let  $X \sim \text{Binomial}(n, \theta)$ , i.e., each try is Bernoulli with probability of success  $\theta$

\* MLE estimator (unbiased):  $\hat{\theta}_{\text{MLE}}(\theta) := X/n$

\* MLE estimator's variance:  $= \text{Var}(X/n) = \theta(1 - \theta)/n$

Consider prior Beta( $a = 1, b = 1$ ) on  $\theta$ , as before.

\* Bayes mean estimator:  $\hat{\theta}_{\text{Bayes}}(\theta) := (X + 1)/(n + 2) = w(X/n) + (1 - w)0.5$

\* Bias of Bayes mean estimator:  $(n\theta + 1)/(n + 2) - \theta = (1 - w)(0.5 - \theta)$

\* Variance of Bayes estimator:  $= \text{Var}(X)/(n + 2)^2 = (\theta(1 - \theta)/n) * (1/(n + 2)^2) = w^2\theta(1 - \theta)/n$

MSE = Bias<sup>2</sup> + Variance

MSE of MLE estimator is mostly (i.e., for most values of  $\theta \in (0, 1)$ ) greater than the MSE of Bayes estimator. Plot.

## Bayesian Cramer-Rao Lower Bound

Applications of the van Trees Inequality: A Bayesian Cramer-Rao Bound

Bernoulli 1995, <https://www.jstor.org/stable/3318681>

Let  $X$  model a dataset.

Consider likelihood  $P(X|\theta)$  with "parameter" / RV  $\theta$

Consider a prior PDF  $Q(\theta|\alpha)$  on "parameter" / RV  $\theta$  with hyper-parameter  $\alpha$

$E_{Q(\theta|\alpha)}[E_{P(X|\theta)}[\hat{\theta}(X) - \theta]^2]$

$\geq$

$$(E_{Q(\theta|\alpha)}[I_P(\theta)] + J_Q(\theta))^{-1}$$

where

$I_P(\theta)$  is the Fisher information of the likelihood associated with PDF / model  $P(X|\theta)$ , and  $J(Q; \alpha)$  is the “prior information” of the prior PDF / model  $Q(\theta|\alpha)$

Unlike the CRLB, the Bayesian-CRLB gives us a lower bound for all (biased and unbiased both) estimators.

Assumption: Consider the prior  $\theta$  defined on (compact) interval  $(a, b)$  such that:

$Q(\theta|\alpha) \rightarrow 0$  as  $\theta \rightarrow a$  and as  $\theta \rightarrow b$

Then, similar to our strategy in proving CRLB, lets consider

$$\begin{aligned} & \int_{\theta=a}^b \int_x \left( \hat{\theta}(x) - \theta \right) \frac{\partial}{\partial \theta} (P(x|\theta)Q(\theta|\alpha)) dx d\theta \\ &= \int_x \int_{\theta=a}^b \hat{\theta}(x) \frac{\partial}{\partial \theta} (P(x|\theta)Q(\theta|\alpha)) d\theta dx - \int_x \int_{\theta=a}^b \theta \frac{\partial}{\partial \theta} (P(x|\theta)Q(\theta|\alpha)) d\theta dx \end{aligned}$$

1st term includes the inner integral:

$$\begin{aligned} & \int_{\theta=a}^b \hat{\theta}(x) \frac{\partial}{\partial \theta} [P(x|\theta)Q(\theta|\alpha)] d\theta \\ &= \hat{\theta}(x) \int_{\theta=a}^b \frac{\partial}{\partial \theta} [P(x|\theta)Q(\theta|\alpha)] d\theta \\ &= \hat{\theta}(x) [P(x|\theta)Q(\theta|\alpha)]_a^b \\ &= 0, \text{ because the prior } Q(\theta|\alpha) \text{ goes to zero at the boundary points } a \text{ and } b \\ & \text{So, the 1st term reduces to zero} \end{aligned}$$

2nd term (without the negative sign) includes an inner integral:

$$\begin{aligned} & \int_{\theta=a}^b \theta \frac{\partial}{\partial \theta} [P(x|\theta)Q(\theta|\alpha)] d\theta = [\theta P(x|\theta)Q(\theta|\alpha)]_a^b - \int_{\theta=a}^b P(x|\theta)Q(\theta|\alpha) d\theta \\ &= 0 - \int_{\theta=a}^b P(x|\theta)Q(\theta|\alpha) d\theta \end{aligned}$$

So, 2nd term (with the negative sign) equals:

$$\begin{aligned} & \int_x \int_{\theta=a}^b P(x|\theta)Q(\theta|\alpha) d\theta dx \\ &= \int_{\theta=a}^b Q(\theta|\alpha) \left( \int_x P(x|\theta) dx \right) d\theta \\ &= 1 \end{aligned}$$

So, our original term equals 1:

$$\begin{aligned} 1 &= \int_{\theta=a}^b \int_x \left( \hat{\theta}(x) - \theta \right) \frac{\partial}{\partial \theta} (P(x|\theta)Q(\theta|\alpha)) dx d\theta \\ &= \int_{\theta=a}^b \int_x \left( \hat{\theta}(x) - \theta \right) P(x|\theta)Q(\theta|\alpha) \frac{1}{P(x|\theta)Q(\theta|\alpha)} \frac{\partial}{\partial \theta} (P(x|\theta)Q(\theta|\alpha)) dx d\theta \\ &= \int_{\theta=a}^b \int_x \left( \hat{\theta}(x) - \theta \right) \sqrt{P(x|\theta)Q(\theta|\alpha)} \sqrt{P(x|\theta)Q(\theta|\alpha)} \frac{\partial}{\partial \theta} \log (P(x|\theta)Q(\theta|\alpha)) dx d\theta \end{aligned}$$

Now, we apply the Cauchy-Schwarz inequality:

$$1 \leq \int_{\theta=a}^b \int_x \left( \hat{\theta}(x) - \theta \right)^2 P(x|\theta)Q(\theta|\alpha) dx d\theta \cdot \int_{\theta=a}^b \int_x P(x|\theta)Q(\theta|\alpha) \left[ \frac{\partial}{\partial \theta} \log P(x|\theta)Q(\theta|\alpha) \right]^2 dx d\theta$$

where

1st integral = expected squared error (NOT variance; because bias of estimator  $\hat{\theta}(x)$  may be non-zero)

2nd integral:

$$\begin{aligned} &= \int_{\theta=a}^b \int_x P(x|\theta)Q(\theta|\alpha) \left[ \frac{\partial}{\partial \theta} \log P(x|\theta) \right]^2 dx d\theta + \int_{\theta=a}^b \int_x P(x|\theta)Q(\theta|\alpha) \left[ \frac{\partial}{\partial \theta} \log Q(\theta|\alpha) \right]^2 dx d\theta \\ &+ 2 \int_{\theta=a}^b \int_x P(x|\theta)Q(\theta|\alpha) \frac{\partial}{\partial \theta} \log P(x|\theta) \frac{\partial}{\partial \theta} \log Q(\theta|\alpha) dx d\theta \end{aligned}$$



where

$$\text{1st term} = \int_{\theta=a}^b Q(\theta|\alpha) \left( \int_x P(x|\theta) \left[ \frac{\partial}{\partial \theta} \log P(x|\theta) \right]^2 dx \right) d\theta = E_{Q(\theta|\alpha)}[I_P(\theta)]$$

$$\text{2nd term} = \int_{\theta=a}^b \left( \int_x P(x|\theta) dx \right) Q(\theta|\alpha) \left[ \frac{\partial}{\partial \theta} \log Q(\theta|\alpha) \right]^2 d\theta = J(Q; \alpha)$$

$$\text{3rd term} = 2 \int_{\theta=a}^b \frac{\partial}{\partial \theta} Q(\theta|\alpha) \cdot \int_x \frac{\partial}{\partial \theta} P(x|\theta) dx \cdot d\theta = 0, \text{ because the inner integral is zero.}$$

Q.E.D.